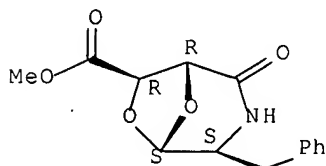


STIC search

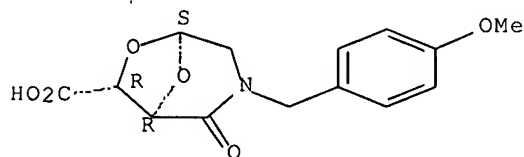
RN 250138-10-4 CAPLUS
 CN 6,8-Dioxa-3-azabicyclo[3.2.1]octane-7-carboxylic acid,
 2-oxo-4-(phenylmethyl)-, methyl ester, (1R,4S,5S,7R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 250138-20-6 CAPLUS
 CN 6,8-Dioxa-3-azabicyclo[3.2.1]octane-7-carboxylic acid,
 3-[(4-methoxyphenyl)methyl]-2-oxo-, (1R,5S,7R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L14 ANSWER 10 OF 11 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1999:580083 CAPLUS Full-text
 DOCUMENT NUMBER: 131:337331
 TITLE: Synthesis and Reactivity of Bicycles Derived from
 Tartaric Acid and α -Amino Acids: A Novel Class
 of Conformationally Constrained Dipeptide Isosteres
 Based upon Enantiopure 3-Aza-6,8-
 dioxabicyclo[3.2.1]octane-7-carboxylic Acid
 AUTHOR(S): Guarna, Antonio; Guidi, Antonio; Machetti,
 Fabrizio; Menchi, Gloria; Occhiato, Ernesto G.;
 Scarpi, Dina; Sisi, Sauro; Trabocchi, Andrea
 CORPORATE SOURCE: Department of Organic Chemistry U. Schiff and Center
 of Heterocyclic Compounds C.N.R., University of
 Florence, Florence, I-50121, Italy
 SOURCE: Journal of Organic Chemistry (1999), 64(20), 7347-7364
 CODEN: JOCEAH; ISSN: 0022-3263
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 131:337331

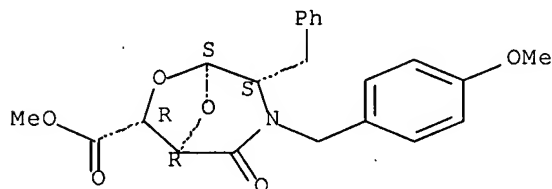
AB 3-Aza-6,8-dioxabicyclo[3.2.1]octane-7-carboxylic acids (named BTAA) derived from (R,R)-, (S,S)-, or meso-tartaric acid and natural (L), unnatural (D), or unusual α -amino acids are described as conformationally constrained dipeptide isosteres. The general strategy developed for their preparation has required the transformation of the amino acids into the corresponding N-benzyl-amino alcs., followed by the PyBroP-promoted condensation with the monomethyl ester of the suitable 2,3-di-O-isopropylidene-tartaric acid. Oxidation of the hydroxy group to aldehyde and subsequent acid-catalyzed trans-acetalization with the two hydroxy groups of the tartaric acid moiety provided 3-aza-2-oxo-6,8-dioxabicyclo[3.2.1]octane-7-carboxylic acid Me esters [named BTAA(O)] in good yield and, in most cases, as single enantiopure diastereoisomers. This strategy has been applied to the preparation of BTAA(O) starting from (R,R)-, (S,S)-, or meso-tartaric acid and glycine, L- and D-phenylalanine, L- and D-alanine, and (\pm)-phenylglycine. In the cases of glycine, L- and D-phenylalanine, and L- and D-alanine, the selective reduction by BH₃·DMS of the amide group succeeding to the cyclization step, or the reduction of both amide and ester functions followed by reoxidn. of the hydroxy to carboxylic group, provided in good yield the 3-aza-3-benzyl-6,8-dioxabicyclo[3.2.1]octane-7-carboxylic acids (or their Me ester) BTAA, having the side chain of the amino acid precursors at position 4. The stability and rigidity of the bicyclic skeleton, the complete control of all the stereo-centers, the possibility of introducing the side chains of L- or D-amino acids, and the demonstrated compatibility with the conditions required for solid-phase peptide synthesis make the BTAA compds. potential dipeptide isosteres useful for the synthesis of modified peptides.

IT 198978-51-7P 250137-79-2P 250137-80-5P
 250137-81-6P 250137-82-7P 250137-84-9P
 250137-85-0P 250137-86-1P 250137-87-2P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and reaction of in the synthesis of 3-aza-6,8-dioxabicyclo[3.2.1]octane-7-carboxylic acid as conformationally constrained dipeptide isosteres)

RN 198978-51-7 CAPLUS

CN 6,8-Dioxa-3-azabicyclo[3.2.1]octane-7-carboxylic acid,
 3-[(4-methoxyphenyl)methyl]-2-oxo-4-(phenylmethyl)-, methyl ester,
 (1R,4S,5S,7R)- (CA INDEX NAME)

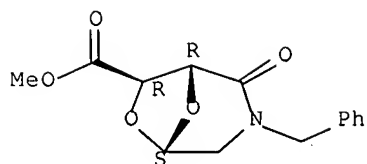
Absolute stereochemistry. Rotation (-).



RN 250137-79-2 CAPLUS

CN 6,8-Dioxa-3-azabicyclo[3.2.1]octane-7-carboxylic acid,
 2-oxo-3-(phenylmethyl)-, methyl ester, (1R,5S,7R)- (CA INDEX NAME)

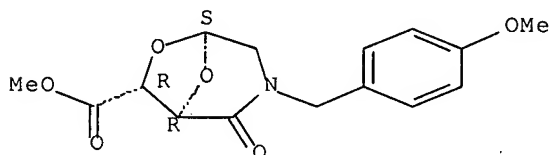
Absolute stereochemistry. Rotation (-).



RN 250137-80-5 CAPLUS

CN 6,8-Dioxa-3-azabicyclo[3.2.1]octane-7-carboxylic acid,
3-[(4-methoxyphenyl)methyl]-2-oxo-, methyl ester, (1R,5S,7R)- (CA INDEX
NAME)

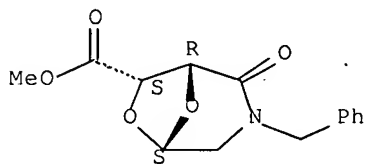
Absolute stereochemistry. Rotation (-).



RN 250137-81-6 CAPLUS

CN 6,8-Dioxa-3-azabicyclo[3.2.1]octane-7-carboxylic acid,
2-oxo-3-(phenylmethyl)-, methyl ester, (1R,5S,7S)-rel- (CA INDEX NAME)

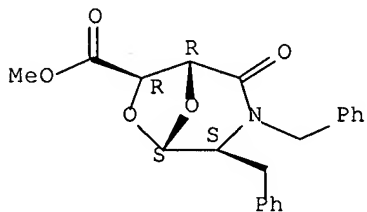
Relative stereochemistry.



RN 250137-82-7 CAPLUS

CN 6,8-Dioxa-3-azabicyclo[3.2.1]octane-7-carboxylic acid,
2-oxo-3,4-bis(phenylmethyl)-, methyl ester, (1R,4S,5S,7R)- (CA INDEX
NAME)

Absolute stereochemistry. Rotation (-).

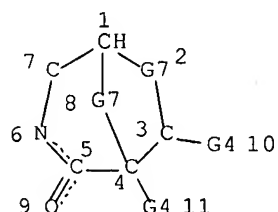


RN 250137-84-9 CAPLUS

CN 6,8-Dioxa-3-azabicyclo[3.2.1]octane-7-carboxylic acid,

SEARCH HISTORY

=> d stat que l12; d his nofile
L9 STR



Ak @12 Ak-Cy
@13 14

VAR G4=H/12/CY/13

VAR G7=O/S/N

NODE ATTRIBUTES:

CONNECT IS E1 RC AT 12

CONNECT IS E2 RC AT 13

DEFAULT MLEVEL IS ATOM

MLEVEL IS CLASS AT 12 13 14

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC 1

NUMBER OF NODES IS 14

STEREO ATTRIBUTES: NONE

L12 225 SEA FILE=REGISTRY SSS FUL L9

100.0% PROCESSED 44361 ITERATIONS

225 ANSWERS

SEARCH TIME: 00.00.03

(FILE 'HOME' ENTERED AT 10:51:09 ON 13 NOV 2007)

FILE 'CAPLUS' ENTERED AT 10:51:55 ON 13 NOV 2007

E US2004-518689/APPS

L1 1 SEA ABB=ON US2004-518689/AP
D SCAN

L2 140 SEA ABB=ON GUARNA A?/AU

L3 41 SEA ABB=ON COZZOLINO F?/AU

L4 21 SEA ABB=ON TORCIA M?/AU

L5 235 SEA ABB=ON GARACI E?/AU

FILE 'REGISTRY' ENTERED AT 10:52:49 ON 13 NOV 2007

L6 STR

L7 7 SEA SSS SAM L6

FILE 'ZCAPLUS' ENTERED AT 10:57:02 ON 13 NOV 2007

L8 7 SEA ABB=ON L7

FILE 'REGISTRY' ENTERED AT 10:57:13 ON 13 NOV 2007

L9 STR L6

L10 6 SEA SSS SAM L9

L11 44361 SEA SSS FUL L9 EXTEND

L12 225 SEA SSS FUL L9

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L13 38 SEA ABB=ON L12

L14 11 SEA ABB=ON (L1 OR L2 OR L3 OR L4 OR L5) AND L13

L15 1 SEA ABB=ON L1 AND L13

FILE 'CAPLUS' ENTERED AT 11:00:09 ON 13 NOV 2007

D QUE NOS L14

D IBIB ABS HITSTR L14 1-11

FILE 'REGISTRY' ENTERED AT 11:00:44 ON 13 NOV 2007

D STAT QUE L12

FILE 'CAPLUS' ENTERED AT 11:00:44 ON 13 NOV 2007

D QUE NOS L13

L16 27 SEA ABB=ON L13 NOT L14

D IBIB ABS HITSTR L16 1-27

FILE 'HOME' ENTERED AT 11:01:07 ON 13 NOV 2007

D STAT QUE L12

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